

April/May 2017

Science & Technology REVIEW

Investment Program Spurs **INNOVATION for 25 YEARS**

Also in this issue:

Projects Explore New Research Avenues

Investigating Optical Damage Initiators

Pillars Add Dimension to Radioisotope Batteries

About the Cover

For more than a quarter century, the Department of Energy's Laboratory Directed Research and Development (LDRD) Program has made possible transformative scientific and technological solutions to ever-changing national security challenges. For example, numerous LDRD projects have supported the research and development of radically new fabrication methods, such as additive manufacturing (AM), to make materials and parts faster, cheaper, lighter, and with entirely novel properties. The cover is an artist's rendering of an octet truss microstructure produced using AM. The geometric configuration is one of the stiffest and lowest weight architectural arrangements for a mechanical structure.



About S&TR

At Lawrence Livermore National Laboratory, we focus on science and technology research to ensure our nation's security. We also apply that expertise to solve other important national problems in energy, bioscience, and the environment. *Science & Technology Review* is published eight times a year to communicate, to a broad audience, the Laboratory's scientific and technological accomplishments in fulfilling its primary missions. The publication's goal is to help readers understand these accomplishments and appreciate their value to the individual citizen, the nation, and the world.

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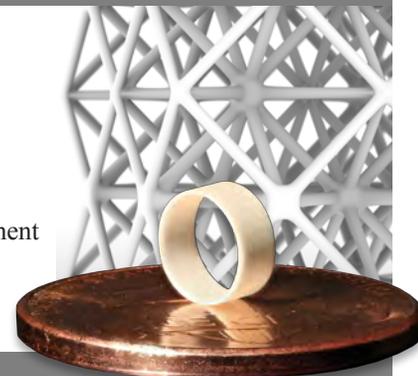
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Elemental Compositions Defy Old Theory

Ten years ago, researchers discovered that rocks on the surface of Earth had a higher abundance of neodymium-142 (^{142}Nd) than did primitive meteorites (also called chondrites). This finding was contrary to the long-standing theory suggesting their chemical and isotopic compositions were the same. The discovery led to a hypothesis that Earth either had a hidden reservoir of neodymium in its mantle or inherited more of the parent isotope samarium-146 (^{146}Sm), which subsequently decayed to ^{142}Nd .

In research appearing in the September 15, 2016, edition of *Nature*, Lawrence Livermore scientists, in collaboration with researchers from the University of Chicago and Westfälische Wilhelms-Universität Münster in Germany, showed the abundance of several Nd isotopes in Earth differ compared to chondrites. Using high-precision isotope measurements, the scientists determined that differences in ^{142}Nd between Earth and chondrites reflected nucleosynthetic processes and not the presence of a hidden reservoir or excess ^{146}Sm . They used large sample sizes (about 2 grams) to obtain improved isotope data for a comprehensive set of meteorites.

According to the team's results, Earth contains Nd that is slightly more enriched by the slow neutron-capture process that occurred during the production of Nd in asymmetric giant branch stars. "The research calls into question a fundamental tenet of geochemistry," says Livermore chemist Lars Borg, who co-authored the paper. "It has tremendous implications for our principal understanding of Earth, not only for determining its bulk composition, heat content, and structure, but also for constraining the modes and timescales of its geodynamical evolution."

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Unprecedented Purification of Copper Nanowires

A team of Lawrence Livermore scientists has developed a new purification method for producing long, uniform, high-purity copper nanowires with unprecedented yields. The research appears in the October 7, 2016, online edition of *Chemical Communications* and was subsequently featured on the cover of the print issue.

The most common approaches to create nanowires also produce byproducts in the form of other low-aspect-ratio shapes, including nanoparticles and nanorods. This difficulty has limited adoption of nanomaterials in many manufacturing technologies. "We have discovered a new approach to efficiently separate copper nanowires from nanoparticles based on their respective surface chemistries. This purification route is a facile, rapid, and inexpensive way to purify different nanomaterials, and it should be broadly applicable," says Lawrence Livermore's Fang Qian, the lead author of the paper. The team demonstrated that copper nanowires, synthesized at liter scale, were purified to near 100 percent yield from their nanoparticle side-products with a few simple steps.

The nanowires and nanoparticles are coated with hydrophobic surfactants and then suspended in an actively agitated mixture of

water and organic solvent. Eventually, the immiscible mixture phase separates, allowing the nanowires to spontaneously cross the interface and separate from the nanoparticles. (See image above.) The team's high-purity copper nanowires meet many of the demanding requirements for potential electronics applications, and the general separation approach provides a possible route to purify industrial-scale quantities of nanomaterials, which remains a key hurdle to the wider commercialization of nanowires. Qian says, "This purification method will open up new possibilities in producing large quantities of high-quality nanomaterials at low cost."

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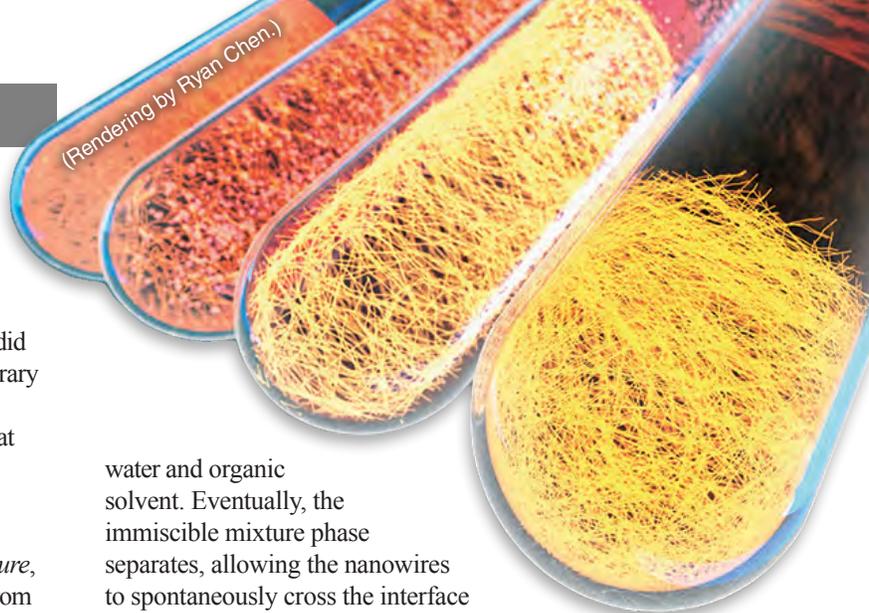
Biomechanical Regulation of a Key Gene in Bone

Researchers from Lawrence Livermore, in collaboration with those at the University of California at Davis and Indiana University School of Medicine, investigated a regulatory element for the gene controlling bone mechanoadaptation—how bone formation responds to pressure loading and unloading. The research appeared in the September 2016 online edition of the science journal, *Bone*.

Over time, pressure loaded on the skeleton builds bone mass, while bone mass is lost from disuse. The gene that expresses sclerostin (*Sost*), a protein that regulates bone turnover, is a negative regulator of bone mechanoadaptation. The study hypothesized that the noncoding enhancer ECR5 was the primary regulatory element, signaling to the *Sost* gene whether it should turn on or off during loading and unloading. Researchers found removing ECR5 did not prevent the effects of unloading on mice with *Sost*. "This finding suggests that ECR5 is not the only regulatory element at play with load-induced regulation of *Sost*. Bone expression is driven by multiple regulatory elements, and the promoter of the gene may be more important than the regulatory element in this situation," says Gaby Loots, a Livermore biomedical scientist and co-author of the paper.

The scientists plan to apply this study's findings toward new research for NASA to help negate the effects of unloading and radiation-induced bone loss in astronauts who spend significant time in space. Astronauts aboard the International Space Station can experience 1–2 percent bone loss per month because of radiation exposure and lack of gravity. Exploring treatment with temporary lack of *Sost* could help overcome these side effects of space travel.

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Celebrating Targeted Investments in Innovative Research

I am pleased that this issue of *Science & Technology Review* is dedicated to the Department of Energy’s (DOE’s) Laboratory Directed Research and Development (LDRD) Program, which is critical to ensuring the continued strength of the Laboratory’s science and technology. The article beginning on p. 4 celebrates 25 years of scientific and technological advances made possible through this program.

By funding innovative research in areas aligned with Lawrence Livermore’s missions, the LDRD Program helps maintain the extremely high quality of our science and technology and ensures we remain the “new ideas” laboratory. The program supports innovative research in areas that have potentially big payoffs but are considered too risky or beyond the planning horizon of our sponsors. In these cases, LDRD investments help us meet emerging mission challenges, attract and retain top researchers, and foster collaborations with other national laboratories, academia, and industry.

As the *Report of the Secretary of Energy Advisory Board’s Task Force on DOE National Laboratories* states, “The ability to adapt, retool, invest in staff and capabilities, and to enter new research areas is crucial to laboratory performance and the maintenance of high-quality staff and research. Laboratories rely in large part on LDRD programs to achieve these goals.” The report cites examples of LDRD research areas including proofs of concept in emerging fields and significant technical solutions that address DOE missions.

Scientific output resulting from LDRD projects, as measured by publications, patents, and invention disclosures, has been prodigious. The *Final Report of the Commission to Review the Effectiveness of the National Energy Laboratories* said it best: “LDRD’s accomplishments are noteworthy. Multiple programs across the system have often begun through initial LDRD investments in capabilities and expertise, and the investments have often produced significant returns—both scientific and financial. In the field of stockpile stewardship, findings of LDRD projects have had a significant impact on stewardship strategy, resulting in dramatic savings to the nation through a more informed understanding of life-extension science.”

Indeed, LDRD programs are particularly important for the three National Nuclear Security Administration (NNSA) laboratories

(Livermore, Los Alamos, and Sandia), which have strict national security–related mission deliverables and schedules. They receive less direct funding for basic science research in areas aligned with their core competencies.

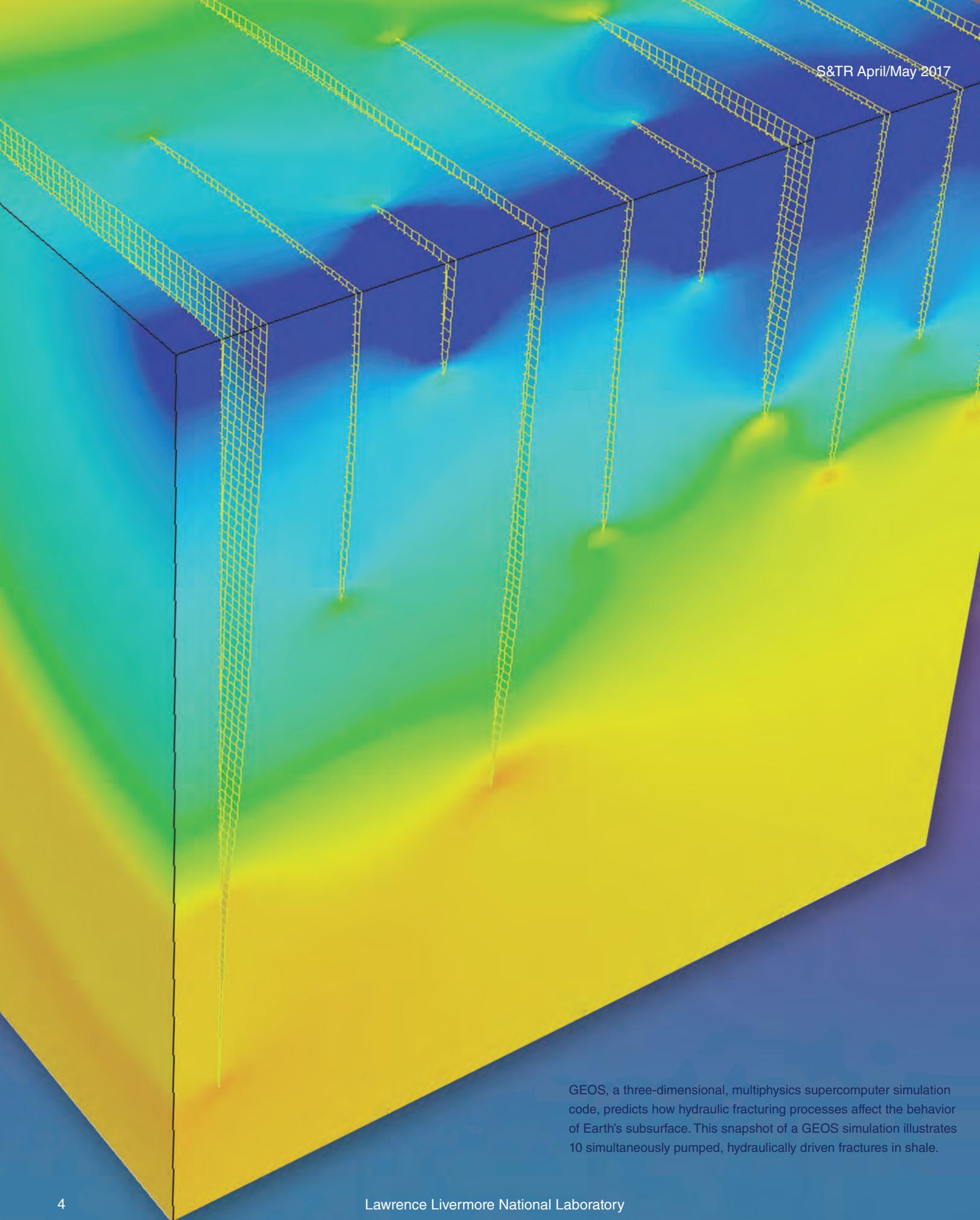
The selection process for individuals to receive LDRD funding is extremely competitive. Every year, proposals and presentations are closely scrutinized by committees composed of senior researchers. Although competition is open to technical staff at all stages of their careers, the program is a valuable component of the Laboratory’s career development strategy. The *Report of the Secretary of Energy Task Force on DOE National Laboratories* also found that for the NNSA laboratories, “LDRD provides a way to maintain a pool of talented individuals whose work is aligned with the core mission of the laboratories.”

The article beginning on p. 13 describes in more detail what the LDRD Program means to career development for our technical staff. Working on an LDRD projects helps to establish early-career researchers in areas of their interest. Early-career scientists also learn how to balance budgets, assign tasks, and administer projects.

LDRD projects cover an exceptionally broad range of national security–related topics, from biodefense to additive manufacturing and from new concepts for National Ignition Facility (NIF) experiments to supercomputing software that aids U.S. oil and gas producers. The two other articles in this issue spotlight LDRD-supported work on radioisotope batteries and on understanding the causes of laser-induced damage to critical optics at NIF.

Over the past several years, the overall LDRD Program has been reviewed by congressional committees, the Government Accounting Office, DOE panels, and external committees. Within the Laboratory, ongoing LDRD research projects are reviewed regularly. Our annual report (<https://lldr-annual.llnl.gov/lldr-annual-2016>) summarizes each project’s scope, motivation, goals, mission relevance, technical progress, and resulting publications. I’m looking forward to another 25 years of outstanding accomplishments, thanks to the LDRD Program.

■ Patricia Falcone is deputy director for Science and Technology.



GEOS, a three-dimensional, multiphysics supercomputer simulation code, predicts how hydraulic fracturing processes affect the behavior of Earth's subsurface. This snapshot of a GEOS simulation illustrates 10 simultaneously pumped, hydraulically driven fractures in shale.

INVESTING IN THE NATION'S FUTURE

The Laboratory Directed Research and Development Program has been a significant engine of scientific discovery for 25 years.

FOR more than a quarter century, the Department of Energy's (DOE's) Laboratory Directed Research and Development (LDRD) Program has yielded an exceptional return on a relatively small investment. Through LDRD funding, Livermore researchers make possible transformative scientific and technological solutions to ever-changing national security challenges.

"LDRD is vital to maintaining the long-term health of Lawrence Livermore's national security mission and its core competencies," says Rokaya Al-Ayat, who is senior advisor to the Laboratory director and also oversees the institution's

LDRD Program. Under LDRD, the Laboratory invests 6 percent of its operating budget (about \$87 million in fiscal year 2017) in areas beyond the scope of programmatic research and where high-risk endeavors could lead to big payoffs. As the Laboratory's primary source of discretionary research and development funding, the program helps maintain the vitality of science and technology disciplines relevant to national security and explores ways to meet future mission needs.

The most innovative science and engineering programs at Livermore often have roots in LDRD. Livermore physicist

Peter Amendt says, "LDRD projects offer the possibility of transformative advances." He adds that these efforts have been effective mechanisms for overcoming difficult physics challenges whose solutions require more time to fully discover the underlying science or technology.

Projects sponsored by LDRD contribute significantly to Lawrence Livermore's intellectual property, publications, and collaborations. The technical output of LDRD researchers—patent disclosures, peer-reviewed publications, and publications cited by other authors—typically accounts for one-quarter of

the Laboratory's total. About half of Lawrence Livermore's patents and 20 percent of published journal articles result from LDRD investments. In the last 10 years, some 60 percent of Livermore's R&D 100 awards have also been attributed to LDRD funding. In addition, many technologies that come out of the LDRD Program have commercial value. The Laboratory's Industrial Partnerships Office licenses these technologies to the private sector to strengthen U.S. industry.

Attracting New Talent

Among the most valuable aspects of the LDRD Program is its role as an outstanding tool for professional growth and recruitment. Projects funded through LDRD are at the forefront of science, helping to attract promising young scientists and engineers. LDRD historically supports more than half of Livermore's postdoctoral researchers, and the projects they work on often influence their career paths. For example, the Laboratory has 15 DOE Early Career Research Program award winners, 14 of whom were supported by LDRD. In addition, 15 of the Laboratory's 23 Presidential Early Career Awards for Scientists and Engineers recipients have been LDRD principal investigators or co-investigators.

LDRD initiatives have proven transformative in all aspects of national security. Four research areas help illustrate the rapid advances possible when a modest investment is made in a talented team of scientists and engineers

Three-dimensional (3D) printing allows researchers to create materials with custom structures, shapes, and mechanical properties while saving time and expense. The microstructures of two different foam materials show (left) a traditional open cell form and (right) a 3D-printed foam with a tetragonal lattice structure.

focused on a new idea. These examples are additive manufacturing (AM), which is revolutionizing the science of how structures are made; new designs, materials, and manufacturing methods for targets used at the National Ignition Facility (NIF); advanced software for improving the efficiency of hydraulic fracturing operations; and the transfer of pathogen-detection technology to industry.

A Manufacturing Revolution

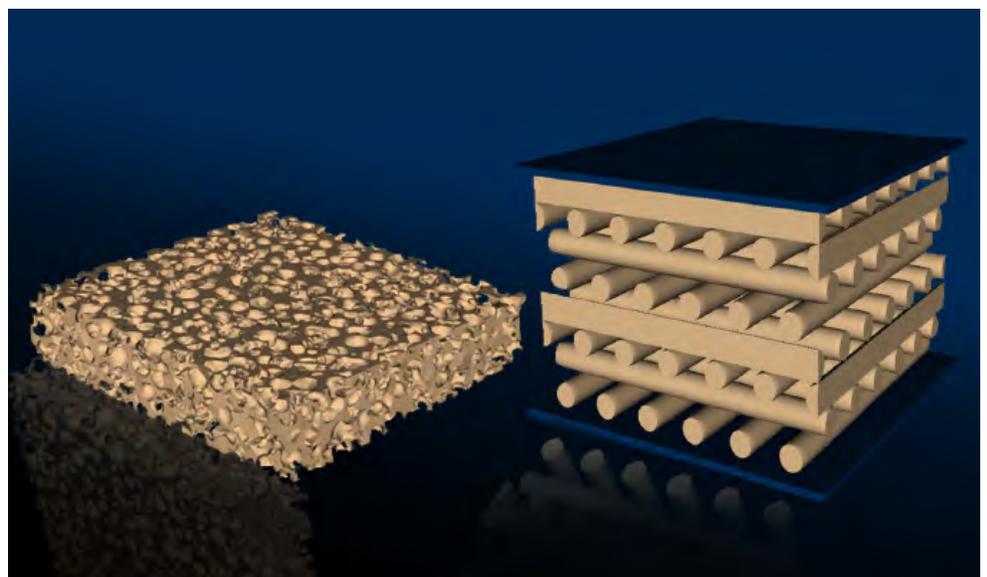
Numerous LDRD projects have supported research and development of radically new methods to make materials and parts faster, cheaper, lighter, and with entirely novel properties. "Many of Livermore's manufacturing and materials solutions have resulted from its LDRD portfolio," says Chris Spadaccini, director of the Laboratory's Center for Engineered Materials and Manufacturing.

AM, often in the form of three-dimensional (3D) printing, typically adds successive layers of material to precisely fabricate 3D objects that may have accompanying complex geometries. Livermore-developed AM technologies, which are revolutionizing manufacturing by producing materials

with unprecedented structural, thermal, electrical, chemical, and photonic properties, are rooted in LDRD. Livermore's focus is to advance those technologies that are not commercially available by integrating manufacturing expertise, precision engineering, materials science, and high-performance computing. The result is innovative multifunctional materials for stockpile stewardship, global security, and energy security.

LDRD-funded projects have led to the manufacture of components incorporating polymers, metals, and ceramics. These parts are produced with reduced cost, less waste, and often remarkably fast turnaround, all of which have greatly accelerated the design-build-test cycle. A materials designer can often produce a prototype part in a few hours, immediately assess its viability, and, if necessary, change a design for improved performance. Indeed, LDRD efforts have demonstrated how components for national security purposes can be produced in weeks to months instead of the several years required using conventional approaches.

In all, LDRD initiatives have resulted in more than 40 AM projects spanning



a broad range of missions. For example, LDRD-driven investments have supported the creation of novel tools such as “optical tweezers” (see *S&TR*, March 2010, pp. 11–13) that use a highly focused laser beam to move microscopic objects, and 3D multibeam lithography, which projects holographic light patterns into photo-curable liquid resins to create 3D structures. Among several new AM processes invented under the auspices of LDRD is laser diode AM (DiAM). A key component of DiAM—now patented and licensed—is the optically addressable light valve. The technology was originally invented by Livermore researchers to shadow defects in valuable NIF optics and prevent further damage.

Innovative modeling and simulation methods for AM have potential for use in stockpile stewardship applications including qualification and certification. An LDRD project headed by Wayne King, leader of the Laboratory’s Accelerated Certification of Additively Manufactured Metals project, is advancing the fundamental understanding of the complex physics behind AM and 3D metal printing. “We want to accelerate qualification and certification of these new materials

and components to take advantage of the flexibility of metal additive manufacturing,” says King.

A stellar example of an AM advance is direct ink writing (DIW), a technique based upon filamentary extrusion of polymer-based “inks.” In 2010, researchers at Livermore collaborated with then University of Illinois Urbana-Champaign professor Jennifer Lewis (now at Harvard University) on an LDRD Strategic Initiative (SI) to adapt the DIW technique. Only two years later, Livermore partnered with the National Nuclear Security Administration’s (NNSA’s) Kansas City National Security Campus to work on manufacturing technologies using DIW.

By 2013, Livermore had designed and procured a unique printing system for making parts with DIW. The following year, Livermore advances were being heralded in international forums and technical journals. The team received an NNSA Award of Excellence in 2015 for exceptional creativity in developing a process for cushions and pads. (See *S&TR*, September 2014, pp. 20–23.) These energy absorbers have tailored mechanical responses and are made with significantly

reduced production time, production footprint, and enhanced production yield combined with improved aging characteristics. Livermore researchers have also used DIW to make engineered graphene aerogel microlattices. This work combines the structural properties of the lattice with the electrochemical functionality of the graphene to form, in one instance, a strong, lightweight, yet compressible high-performance supercapacitor. (See *S&TR*, April/May 2015, pp. 14–18.)

The most visible result of the impressively rapid rise of LDRD-supported AM science is the 13,000-square-foot, \$9.4 million Advanced Manufacturing Laboratory at the Livermore Valley Open Campus. (See *S&TR*, March 2011, pp. 22–25.) This facility, now under construction, will provide a space for Livermore employees to collaborate with industry and academic partners on AM technologies. Spadaccini says that initial LDRD support of AM research helped expand the method’s possibilities, which has led to support for such a facility.

The growing AM effort has attracted talented scientists and engineers to Livermore, including more than 40 postdoctoral researchers and 60 summer interns over the past 6 years. Livermore researchers have also been collaborating with graduate students at universities across the nation on related efforts. In this area, more than 80 invention disclosures and 50 patents have been filed. Moreover, upwards of 10 Cooperative Research and Development Agreements (CRADAs) and industry-related projects are under way.

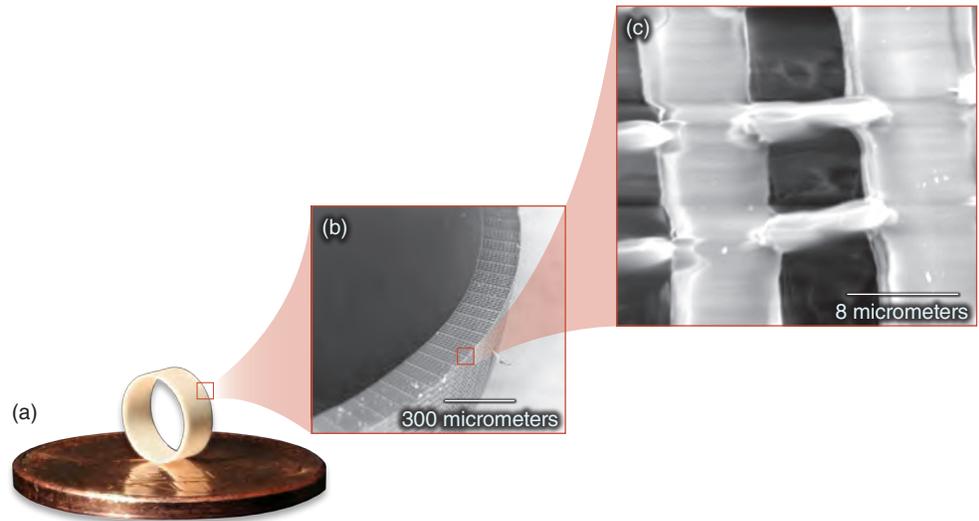


Livermore engineers Eric Duoss (left) and Tom Wilson use an additive manufacturing process called direct ink writing to develop an engineered porous cushion. (Photo by George A. Kitrinos.)

Improved Target Fabrication

NIF experimental targets, typically no larger than a few millimeters in diameter, include two broad categories: high-energy-density (HED) physics targets that test materials at nuclear weapons-related extreme temperatures and inertial confinement fusion (ICF) targets aimed at furthering the understanding of laser fusion. LDRD investments in fabricating both types of targets have resulted in substantial contributions to both materials science and national security.

Before NIF began operation in 2009, two three-year-long LDRD SIs, one begun in 2005 and the other in 2008, were highly successful in establishing new designs and manufacturing capabilities for advanced laser targets. These two efforts were conducted under the auspices of Livermore's Nanoscale Synthesis and Characterization Laboratory (NSCL). Under the SIs, researchers greatly advanced the science and engineering needed to produce nanocrystalline grains, nanoporous foams, high-strength aerogels, atomic-layer deposition techniques, advanced lithography, and joining techniques for precision microassembly. Alex Hamza, former NIF target fabrication manager and now director of the NSCL, says, "The impact



Using the two-photon polymerization direct laser writing technique, a Livermore research team manufactured (a) a hohlraum foam liner template. Scanning electron microscopy images show the liner magnified (b) 230 and (c) 10,000 times. The liner's thickness, density, and composition were specifically "tuned" by the on-demand fabrication process.

on the materials science community was enormous. The two SIs resulted in technical papers that have been cited more than 8,000 times."

Amendt notes that the contributions from the first SI alone continue to yield dividends. Many advancements have been adopted by Livermore programs, while other efforts are being pursued in subsequent LDRD efforts. For example, scientists devised a prototype double-shell ICF target as a test bed for integrating new materials and methods. The double-shell design is a complementary approach to the traditional single-shell target. Early experimental results have been encouraging.

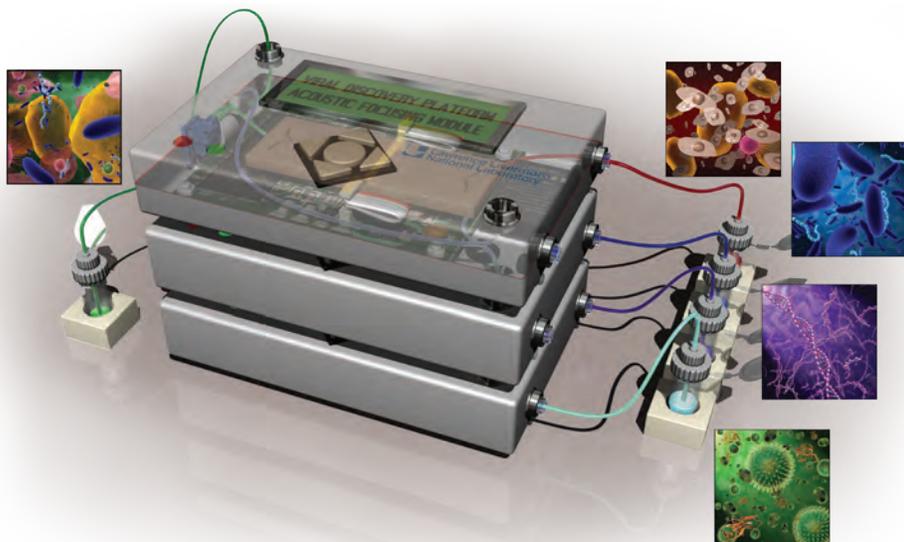
An SI breakthrough, accomplished with the collaboration of Diamond

Materials and General Atomics, was a high-strength diamond capsule to replace plastic ablator shells. A key advantage of diamond over plastic is its roughly three times higher density, permitting diamond ablator shells to be only one-third the thickness of plastic ones. Diamond shells can also be fabricated with extremely smooth surfaces. Together, these advantages result in better confinement of deuterium-tritium (DT) fuel. Hamza says, "Diamond capsules for both ICF and HED targets are now regularly used at NIF."

Other LDRD-fostered ideas have included changing the design of the hohlraum, a tiny metal casing open at both ends that encloses the NIF target. A candidate design is a rugby hohlraum, which resembles a cylinder with the corners rounded off to minimize surface area. The hohlraum's oblong shape helps

Rugby hohlraums (one-half of a prototype is shown here) resemble a traditional cylinder-shaped hohlraum, but with the corners of the cylinder rounded off. Laser light enters the casing through both ends, and the rugby design reduces energy loss in the walls because of their smaller surface area.





An artist's concept shows the viral discovery platform Livermore researchers developed to separate viruses from other sample materials, such as bacteria, mammalian cells, free DNA, and proteins. The work was done as part of a Laboratory Directed Research and Development project to more rapidly identify and characterize pathogens. (Renderings by Kwei-Yu Chu and Sabrina Fletcher.)

reduce energy losses that typically occur through a hohlraum's wall surface.

One of the biggest payoffs from LDRD investments in target designs, fabrication methods, and materials was new techniques to produce nanoporous foams—extremely lightweight porous structures made from different materials with uniformly sized holes at the nanoscale. Researchers have created an entire suite of low- to high-Z (atomic number) foams, including those with graded densities. A DT-saturated polymer foam developed over the last decade is designed to replace the thin layer of DT “ice” typically used in ICF experiments.

LDRD funding also led to the development of the polyelectrolyte enabled liftoff (PEEL) technology, which can fabricate polymer films that are larger, stronger, and thinner than those produced with conventional methods. The extremely thin (about 6 nanometers or 30 atoms thick) PEEL-produced membranes serve as “tents” for suspending ICF fuel capsules inside hohlraums. PEEL was named one of the

top 100 industrial inventions worldwide for 2016 by *R&D Magazine*. (See *S&TR*, January/February 2017, pp. 16–17.)

Advances in AM developed through LDRD investments are further empowering target fabricators. An LDRD-funded team led by Livermore's Juergen Biener is accelerating fabrication time from weeks to hours for polymer foam and aerogel components used in targets. The “on demand” capability allows researchers to easily change a material's properties, such as density, elasticity, and brittleness, and parts can be 3D printed with specified properties, structure, and shapes. Biener says, “With AM technology, we are independently controlling the surface area, pore size, and pore volume of our aerogels.”

Another idea borne out of LDRD investments is incorporating a foam liner into a hohlraum to improve implosion symmetry. Through an AM process called two-photon polymerization direct laser writing, Biener's team fabricated the first millimeter-sized, low-density foam parts with nanoscale features for

material strength tests and as hohlraum liner templates. The breakthrough production methods can also be applied to sustainable energy applications such as hydrogen and electrical energy storage. In another example, LDRD funding laid the foundation for creating an on-chip material library of nanoporous gold structures for studying the relationships of structures and properties, such as those of neural interfaces. “We're still reaping the benefits of LDRD investments that ended seven to ten years ago,” says Hamza.

New Ways to Identify Pathogens

LDRD investments have long supported the development of new approaches for rapid and accurate detection of biological agents that could be unleashed by rogue nations and terrorist groups. Half of Lawrence Livermore's royalties from licensing agreements are from novel technologies developed within its biotechnology program, and LDRD has been the seedbed for many of these commercial successes. A particularly notable technology transfer success was the formation of QuantaLife, Inc., which converted an LDRD-developed technology aimed at detecting dangerous pathogens to commercial medical applications.

Two long-term Livermore employees, Bill Colston and Fred Milanovich, left the Laboratory in 2008 to found QuantaLife and develop sensitive and accurate commercial genetic-testing products based on Livermore-developed pathogen-detection technology. Specifically, QuantaLife licensed digital polymerase chain reaction (PCR), a refinement of real-time PCR, which allows researchers to quickly identify extremely low concentrations of pathogens contained within a sample.

The key technology was what QuantaLife called droplet digital PCR (ddPCR). For years, scientists had solely used traditional PCR to identify

the genetic composition of a specimen. However, this technique can miss extremely small amounts of DNA or RNA that signal the presence of a pathogen. With ddPCR, the sample is split into a large number of equivalent droplets, and then traditional PCR is carried out in each partition. In this way, ddPCR detects rare DNA that might typically be lost in the background.

The ddPCR technique had its origins in an LDRD project called the viral discovery platform. The project, led by Chris Bailey, focused on development of a new approach for rapidly identifying and characterizing viruses in liquid samples. Bailey's team leveraged Livermore advances in microfluidics (manipulation of liquids in tiny channels) and demonstrated microfluidic isolation of virus particles in complex biological samples. The team also developed the first-ever bioinformatics (software to analyze biological data) system that optimized pathogen signatures (regions of DNA unique to a species) for rapid identification. Another

advancement was the team's creation of the first comprehensive, automated sample-preparation system for sorting all components in clinical samples. Furthermore, the LDRD effort advanced the technology of microarrays, where gene sequences are placed onto a chip to detect pathogens.

"Biological samples are messy and complicated. Our aim was to develop a platform where we could isolate low concentrations of pathogens and identify them," says Bailey. "Typically, scientists are looking for only one pathogen, but we developed a technique that could test for many different pathogens. We brought together various technologies to get a deeper view of what a biological sample contained. We were successful because we had such diverse capabilities at the Laboratory, especially bioinformatics, which is critical to analyzing complex samples and generating unique signatures."

The third generation of the microbial discovery platform contained bacterial and fungal signatures in addition to

those for viruses, making it the most accurate and sensitive genetic analysis platform for pathogens developed at the time. The system was tested on various samples, including those from paralyzed children in Pakistan and sick sea lions living on the California coast. The system was also used to check the purity of a commercially available rotavirus vaccine. The platform detected contamination from a porcine virus. Subsequently, sales of the vaccine were suspended until it could be proven safe.

With the help of Livermore's Industrial Partnerships Office, QuantaLife gained the rights to commercialize the Livermore technology and apply a breakthrough originally developed for national security to clinical medicine. Colston helped grow QuantaLife into a company of more than 60 employees by 2011. During his Livermore career, Colston headed the Biodefense Knowledge Center, led the Chemical and Biological Countermeasures Division, secured 13 patents, and received three R&D 100 awards. Co-founder Milanovich directed the Laboratory's Chemical and Biological National Security Program, and in 2002 was named a Lawrence Livermore Edward Teller Fellow. Both founders were also inducted into the Laboratory Entrepreneurs' Hall of Fame.

QuantaLife was honored as the "most promising company" at the Personalized Medicine World Conference in 2010. Later versions of ddPCR earned the Best New Life Sciences Product in 2013 and a Federal Laboratory Consortium Outstanding Commercialization Success Award. In 2011, Bio-Rad, Inc., acquired

Lawrence Livermore Director Bill Goldstein (left) congratulates former Livermore employee Bill Colston on his election to the Laboratory Entrepreneurs' Hall of Fame. Colston co-founded QuantaLife, Inc., which commercialized a breakthrough Livermore technology for detecting and identifying pathogens.



QuantaLife for \$162 million. Bio-Rad continues to enhance the product. Bailey says, “We developed the technology for national security, but QuantaLife made it useful for medicine.”

Enhanced Hydraulic Fracturing

A major element of national security is energy security, and LDRD-supported efforts have helped to reduce U.S. dependence on imported oil. Hydraulic fracturing, also known as hydraulic stimulation, has revolutionized domestic hydrocarbon production and is providing the nation with an abundant source of oil and natural gas.

Fractures produced or reactivated during hydraulic stimulation provide an efficient pathway for the transport of hydrocarbons that are tightly bound within rock and wellhead. The process was initially developed in the 1980s and 1990s with the help of DOE funding. A typical hydraulic fracturing well begins as a vertical well that is subsequently steered to penetrate horizontally for many kilometers. A combination of water, viscous fluids, and sand is then pumped into the well at high pressure, opening fractures that liberate oil and gas.

However, hydraulic fracturing operations typically recover only a small portion of the available oil and gas, and energy producers wanting to maximize production struggle to understand the physical mechanisms that govern the hydraulic stimulation. In addition, longstanding concerns remain regarding the large amounts of water routinely used in the process, the potential contamination of aquifers, and the triggering of seismicity from water reinjection.

To increase hydraulic fracturing efficiency, decrease costs and environmental impacts, and enhance understanding of the hydraulic stimulation process, a Livermore team, funded by LDRD, developed GEOS, a 3D multiphysics supercomputer

A Rigorous Selection Process

Livermore scientists and engineers who seek funding from the Laboratory Directed Research and Development (LDRD) Program must choose from among four project categories: Strategic Initiative (SI), Exploratory Research (ER), Laboratory-Wide (LW), and Feasibility Study (FS). SIs involve large multidisciplinary, cross-organizational teams and are funded for up to three years at \$1.5 to \$3 million per year. ERs represent investments in core competency areas and are funded typically for less than \$1.5 million per year. LWs are small projects that serve as incubators for proposals from early-career personnel. (See “Program Supports Blazing New Trails,” beginning on p. 13 of this issue.) FSs are funded at less than \$175,000 for one year, but are considered for funding opportunities throughout the year.

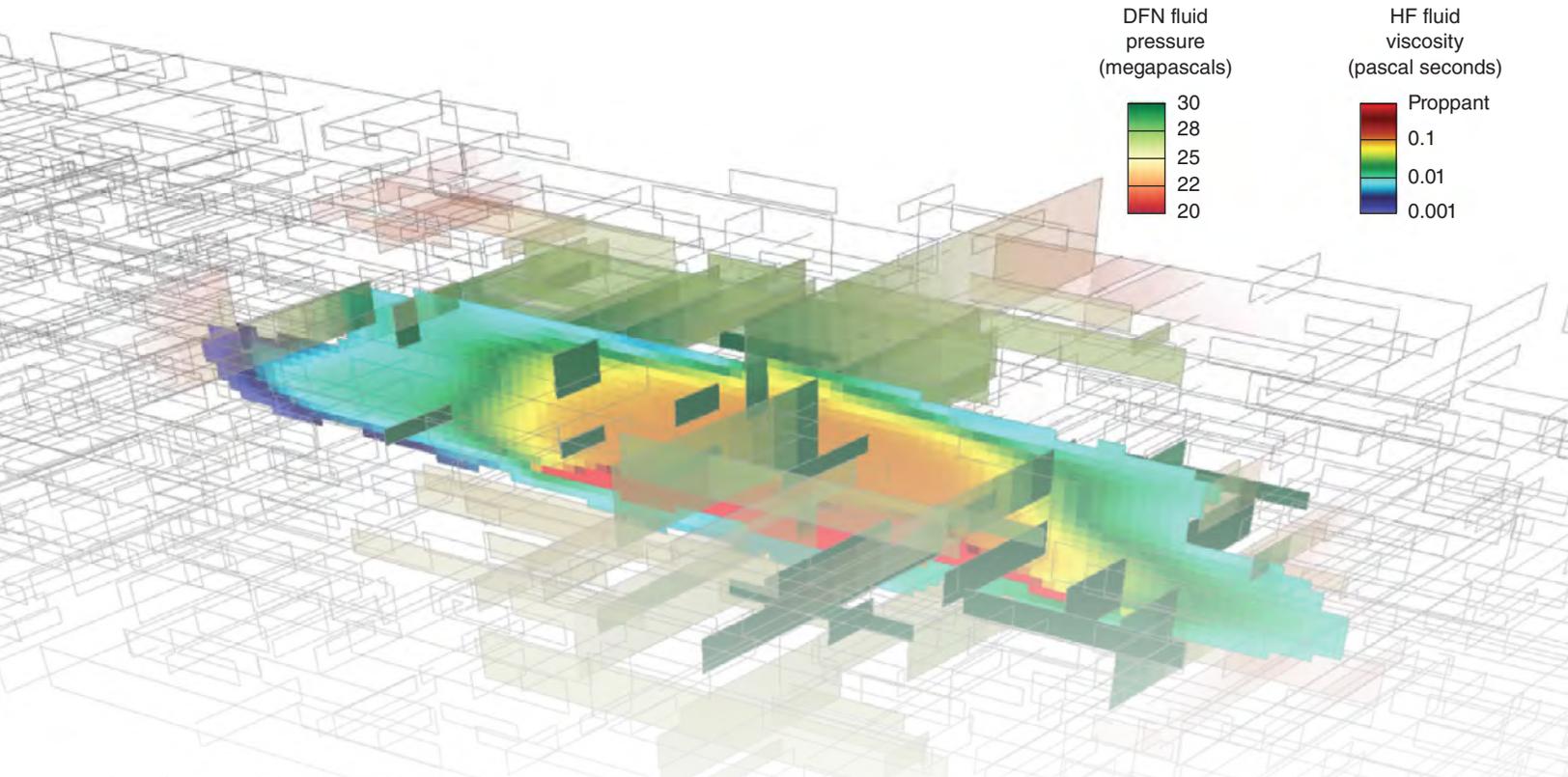
During the first quarter of each calendar year, the Laboratory director issues a call to all scientific and technical personnel for LDRD proposals in the four project categories. All proposals are rigorously evaluated with criteria consistent with those used across the scientific community, in particular the National Science Foundation and the National Institutes of Health. Scientific and technical merit is a key element of the review process, as are innovation and creativity, potential impact on the technical field, qualifications of the researchers, available resources, and the proposed research approach.

simulation code. GEOS is a powerful tool for predicting the behavior of Earth’s subsurface and guiding oil and natural gas extraction from shale formations, thereby maximizing the yield of underground reservoirs.

“Conventional practices leave so much oil and gas in the ground that even a small increase in efficiency helps,” says lead GEOS developer Randolph Settgast. He notes that well operators have limited information about how the rock fractures they create will form and propagate when subjected to high-pressure fluid injections. GEOS incorporates models of the physical processes that accompany hydraulic stimulation and control the formation and propagation of fractures. Using reservoir models representing the heterogeneous nature of the subsurface, GEOS predicts the response to stimulation, including the lateral and vertical extent of the fracture as well as its shape and aperture. GEOS simulates the growth of fractures over a spatial range extending kilometers—from near the well to the entire reservoir—and spans a temporal scale ranging from seconds to years. In this way, the

code helps operators to more efficiently exploit the subsurface layer containing the most natural gas or oil. For example, the code seeks to guide decisions on the optimum spacing of production wells and recommend the best pumping schedules.

GEOS’ development effort, which began under a 2011 LDRD SI led by geophysicist Rick Ryerson, took advantage of Livermore expertise in computational geoscience, high-performance computing, mechanical engineering, geomechanics, seismology, hydrology, and the experience of industrial partners. Currently, three GEOS-related LDRD initiatives are under way. One team, led by Joseph Morris, is modeling “dynamic stimulation,” in which energetic materials are used to enhance hydrocarbon production in tight formations. Another LDRD group is analyzing stress and strain data from fiber-optic acoustic sensors inside a well to better characterize fracturing operations. A third team, led by Pengcheng Fu, is performing simulations to advise California’s Division of Oil, Gas, and Geothermal Resources on the efficiency and environmental impacts



A GEOS simulation shows the growth of fractures caused by a horizontal hydraulic fracturing well pumping fluid into an oil-containing layer of subsurface shale. Color gradients correlate to the discrete fracture network (DFN) fluid pressure and hydraulic fracture (HF) fluid viscosity. The full duration of the simulation is 102 minutes, about the time it takes to stimulate a 300-meter-long section of a production field.

of cyclic steam injection and hydraulic stimulation in California oil reservoirs.

Livermore researchers are also working with colleagues at Lawrence Berkeley National Laboratory as part of DOE’s Exascale Computing Project to couple the GEOS code with a Lawrence Berkeley code that simulates pore-scale flow and geochemical reactions of fluids. Settgest explains, “Together, the coupled codes will allow us to simulate the performance of a vertical well ranging from the flow and chemistry of fluids in rock pores to large-scale fractures.”

Two CRADAs, one with a small independent company and the other with a major oil producer, are aimed at validating the performance of GEOS under real-world conditions. Settgest says that working closely with the oil and gas companies has helped the group refine its goals. “The companies are looking for partners they can trust,” he says. “They know the LDRD efforts are nonprofit, and we are upfront about the capabilities we do and do not have.” GEOS is poised to become an important tool for energy security. The code could also be used

to enhance operations at geothermal power plants.

Celebrating 25 Years of Success

With LDRD making possible national security advances on so many fronts, competition among scientists and engineers for this prized funding source remains fierce. (See the box on p. 11.) LDRD projects are selected on a highly competitive basis through rigorous management and peer-review processes, and only 1 in 10 proposals receives funding. However, researchers whose proposals are turned down receive valuable feedback about their submittals and are encouraged to apply the following year.

Applicants say that despite the intense competition for obtaining LDRD funding, the opportunity to pursue frontier science—and make an important research contribution—makes the effort more

than worthwhile. LDRD-funded efforts have produced enormous payoffs from modest investments over the past 25 years. Another quarter century of outstanding results is just beginning.

—Arnie Heller

Key Words: additive manufacturing (AM), Center for Engineered Materials and Manufacturing, Cooperative Research and Development Agreement (CRADA), Department of Energy (DOE) Early Career Research Program, direct ink writing (DIW), droplet digital polymerase chain reaction (ddPCR), Exascale Computing Project, GEOS, hohlraum, hydraulic fracturing, Laboratory Directed Research and Development (LDRD) Program, Nanoscale Synthesis and Characterization Laboratory (NSCL), National Ignition Facility (NIF), polyelectrolyte enabled liftoff (PEEL), Presidential Early Career Awards for Scientists and Engineers, QuantaLife, Inc.

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Program Supports **BLAZING NEW TRAILS**

SCIENCE can make leaps in progress when researchers explore innovative ideas summoned from the deepest wells of their creativity. Lawrence Livermore's Laboratory Directed Research and Development (LDRD) Program (see "Investing in the Nation's Future" beginning on p. 4 of this issue) encourages these "out-of-the-box" endeavors through its Laboratory-Wide (LW) category of projects. LWs are small projects that serve as incubators for proposals from early-career personnel. The funding allows these researchers to perform research that may not precisely align with Livermore's investment strategy, but which is relevant to the institution's missions. Such projects have potential to open new avenues of investigation and enable novel approaches to achieving mission objectives.

LW LDRD projects have helped a generation of Laboratory scientists establish their careers, and in some cases, research directions that become their life's work. These projects have also taught them how to propose and present research proposals to a funding body and to organize and manage all aspects of a research effort, from overseeing the work and balancing budgets to assigning tasks and performing project administration. "The stronger our LDRD principal investigators (PIs) are, the stronger we are as an institution," says Eric Gard, chairperson for the LW LDRD portfolio. "Through Laboratory-Wide projects, we are attempting to prepare our people and their technologies for the real world. This category of research helps scientists develop the technical skills they need to succeed in science."

To receive LW LDRD funding, a researcher must submit a written proposal, which is evaluated by a review committee. If the proposal makes the cut, the researcher must then make an oral presentation. LW LDRD projects are extremely competitive, and thus winning one is a major achievement. PIs are provided a maximum of \$300,000 per year for two years. Awardees can obtain funding for an additional third year, but they must compete with new LW proposals and prove that the extra time is needed. The LDRD Program offers coaching to help submitters write their initial funding proposals and, if they are selected, prepare for their subsequent oral presentations in front of the review committee.

A Compact X-Ray Source Sees First Light

Physicist Félicie Albert is one Livermore scientist for whom LW LDRD funding made a difference. “Support through the program was game-changing,” she says. “It allowed me to explore scientific ideas I would not have been able to investigate otherwise and to form collaborations with universities. It was also critical to my winning a Department of Energy Early Career Research Program (ECRP) award.” The ECRP award is a prestigious grant that offers young investigators five years of funding up to \$2,500,000.

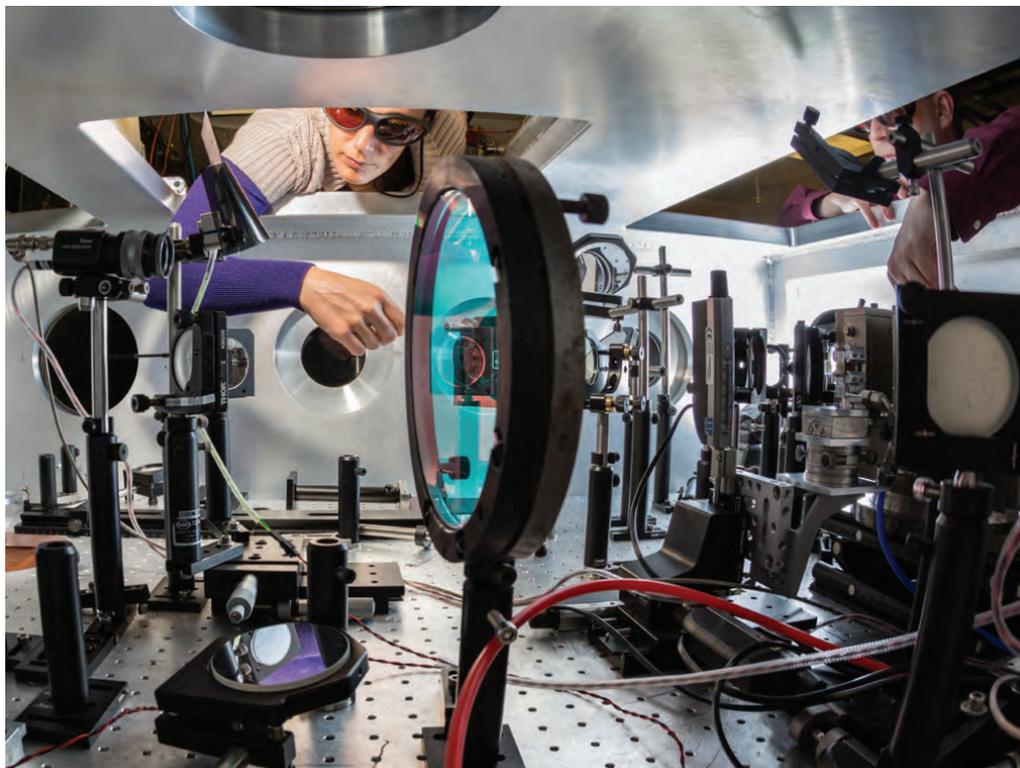
Albert and her team developed a compact hard x-ray source to study phenomena in the high-energy-density (HED) regime (extremely high temperatures and pressures) and characterize materials. Using an ultrahigh-intensity, extremely short laser pulse directed into a gas-filled cell, high-energy x rays are produced by electrons accelerating within the wakefields of laser-produced plasma, eliminating the need for a particle accelerator-sized machine to create the intense radiation. (See *S&TR*, January/February 2014, pp. 16–18.) This compact x-ray source will help Livermore continue its stockpile stewardship mission, advance fusion energy science, develop advanced materials, and probe the nature of matter. With further development, laser wakefield-based x-ray sources

may someday be useful for medical imaging. “The LW LDRD project gave me the credibility to prove that the source works,” says Albert. With her ECRP award, Albert is expanding the tool to perform HED experiments at large-scale science facilities.

A More Realistic Look at Pathogens

Viruses, the causal agent behind many difficult-to-cure diseases, readily reproduce within live hosts. Viruses mutate quickly, presenting a moving target, and making viral diseases difficult to treat. Scientists have been slow to develop successful antiviral therapies because studies of viruses in laboratory animals are expensive. Many studies make do with culturing viruses in flasks, but the pathogens and the cells they infect last only a few days—too short to follow them through multiple mutations.

LW LDRD funding offered Livermore engineer Maxim Shusteff, an expert in microfluidic technology, to apply his expertise toward developing a new technology that could have a substantial benefit on a significant scientific problem—how to culture viruses in a realistic environment to study their mutations and develop effective therapeutic agents. Through his LW LDRD project, Shusteff and his collaborators at the University of California at San Francisco have developed a technology to allow viruses to infect tissues in a steady-state, cell-culturing platform. This platform allows the team to continuously introduce new cells into and remove



Livermore researchers Félicie Albert (left) and Bradley Pollock prepare the tabletop-sized Callisto laser system for laser-wakefield, high-energy x-ray experiments at the Laboratory's Jupiter Laser Facility.

older virus-infected cells from a tissue culture. First, viruses infect mammalian cells in a bioreactor. An acoustic separator then filters out free virus particles, allowing the infected cells and viruses to be extracted separately for genetic sequencing and analysis, while fresh media, and, if needed, new, uninfected cells, flow into the bioreactor. Shusteff says, “Our system controls the cell population continuously and allows the tissue-infection process to proceed in a more lifelike way.”

LW LDRD funding let Shusteff investigate the potential of this technology and the scientific context where the device could be helpful. “Great ideas for a technology have to address an important scientific space,” he says. Having completed the third year of his LW LDRD, Shusteff’s team is looking forward to culturing the cells of multiple organs and biological systems—for instance, the lungs and the immune system—for study in his viral platform.

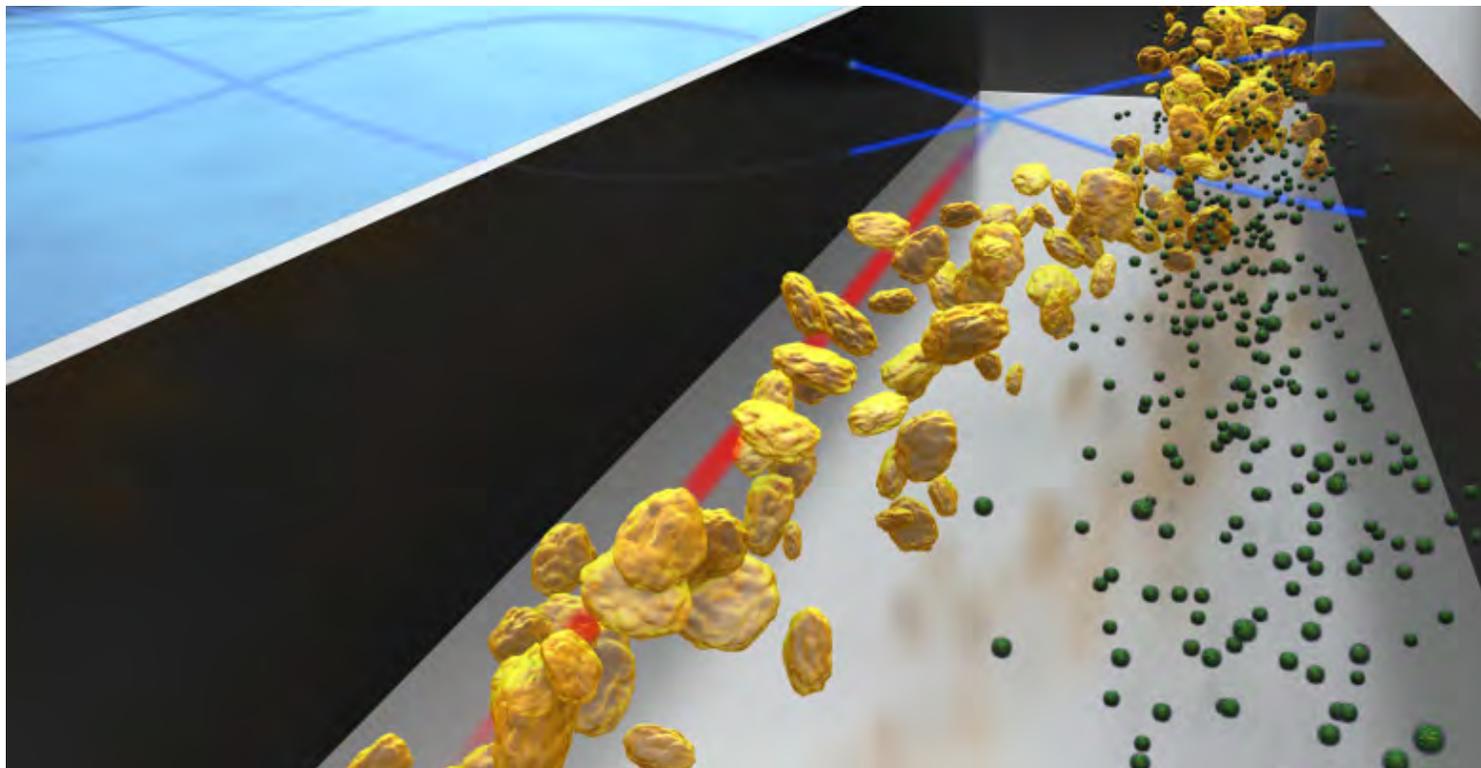
Career-Changing Research

Livermore scientists who obtained LW LDRD funding early in their careers speak glowingly of its influence on establishing their research directions. “The program was pivotal to my career at Livermore,” says Erik Draeger, now group leader of Livermore’s High-Performance Computing Group in the Center for Applied Scientific Computing. “My mentor at the

time encouraged me to explore a project outside the scope of my postdoctoral work. It was a useful exercise for me to go through the process of developing a written proposal and a presentation—even if I didn’t win.” But win one he did, and in 2004 he set out to develop a molecular dynamics simulation of the human P450 CYP1A2 enzyme, which plays an important role in mediating the effects of carcinogens in the body.

The simulations required developing a hybrid of classical and quantum dynamics methods. Although trained in theoretical condensed matter physics, Draeger began focusing on computational biology because of this project. “I discovered that my passion was creating new capabilities to help make scientific discoveries possible,” he says. Draeger went on to work on a supercomputer code called Cardioid that realistically

Livermore scientist Maxim Shusteff is developing a steady-state, cell-culturing platform for viruses. A rendering of the technology shows cells (yellow) and viruses (green) being separated by an acoustic field (blue lines). Fluid flow is toward the viewer, with a stream of mixed particles entering the device side-by-side with a clean fluid stream. The acoustic field moves the cells toward the pressure node (red line) and into the clean fluid, while the undeflected viruses continue straight, exiting the device through a separate outlet (not shown). (Rendering by Kwei-Yu Chu.)

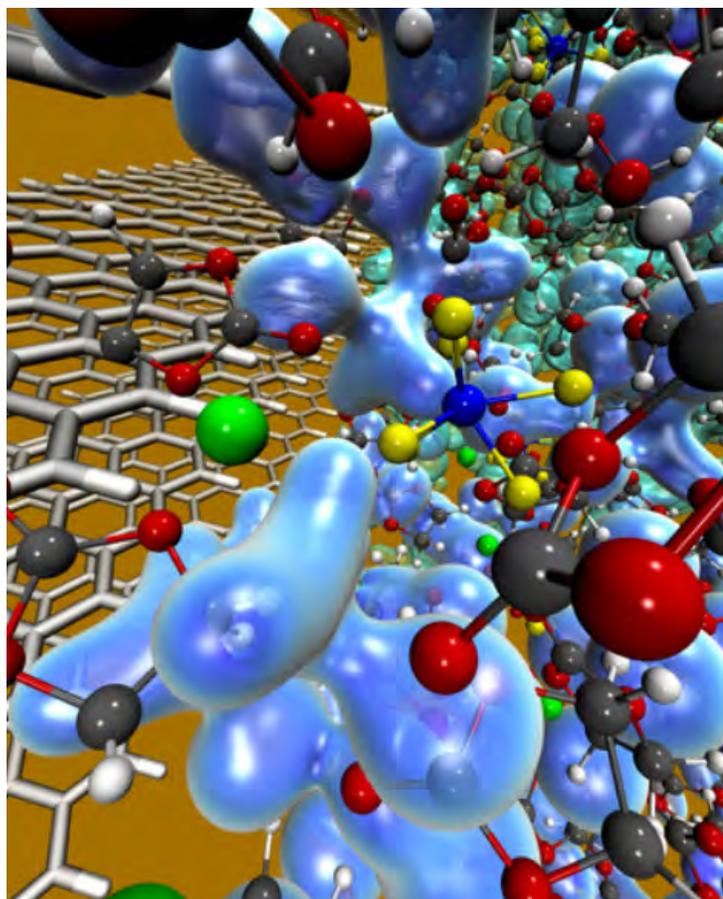


mimics the electrophysiology of a beating human heart. He has also continued to develop Qbox, a first-principles molecular dynamics code that uses density functional theory to compute the electronic structure of atoms, molecules, solids, and liquids.

In 2015, Draeger became a mentor to then Lawrence Scholar Amanda Randles, and seeing the benefit of LW LDRD research, encouraged her to propose her own project. After winning the funding, she began her endeavor to validate large-scale fluid dynamics simulations of objects with complex geometries. The intent of the project was to adapt three-dimensional (3D) printing to create objects that accurately replicate biological structures, such as the circulatory system. First, the project team

extended a code called Harvey to simulate fluid flow through blood vessels. Then, the Livermore researchers collaborated with a team at Arizona State University (ASU), which 3D-printed blood vessels, such as the aorta, and measured their fluid dynamics. The Livermore team validated Harvey against ASU's observations of the printed blood vessels.

Randles is now an assistant professor of biomedical engineering at Duke University, where she is establishing a laboratory to use computational tools for studying the evolution of diseases such as atherosclerosis and cancer. She says, "The LDRD project was essential to validating the Harvey code. It helped us demonstrate that the code provided similar velocity profiles to what was discovered in the experiments—even for highly turbulent flow." As with Draeger, Randles' project also provided her with a new career path. "Although I was trained in physics and computer science, the LW LDRD work enabled me to move into biomedical engineering." From her post at Duke, she continues to collaborate with Draeger, as well as with Livermore biomedical engineer Monica Moya, who is working on an LDRD to create a full vascular system using 3D printing. (See *S&TR*, March 2016, pp. 13–16.)



Qbox is a first-principles molecular dynamics code written to carry out large simulations on massively parallel supercomputers. This image is taken from a 25-picosecond, 1,700-atom simulation of a lithium-ion cell anode–electrolyte interface. Livermore computational scientist Erik Draeger continues developing the open-source Qb@ll version of the code.

A Beneficial Endeavor

According to Draeger, one of the major benefits of the LW LDRD process is learning how to sell an idea. "Not everyone understands why the proposed research is important. When a scientist or engineer is in front of the selection committee, that person must prove the project's significance to the reviewers. Learning how to communicate, how to tell your story convincingly, is an important skill."

To current and future Laboratory researchers who seek to broaden their research horizons and scientific reach, the LW LDRD projects are a prime avenue to follow. However, not every attempt at funding yields success. Albert focuses on not giving up, echoing advice that is a universal feature of success: "If you have a good idea, be persistent. It took several tries before I won my LDRD—but the reward is well worth the time and effort you put into it."

—Allan Chen

Key Words: bioengineering, bioreactor, Cardioid, cell culture, compact x-ray source, Department of Energy Early Career Research Program (ECRP), high-energy-density (HED) science, Laboratory Directed Research and Development (LDRD) Program, Laboratory-Wide (LW) LDRD, laser wakefield, microfluidics, molecular dynamics, plasma, Qbox, therapeutic agent, tissue culture.

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LOOKING for TROUBLE on Optical Surfaces

HIGH-ENERGY pulsed lasers, including the world's most energetic laser at Lawrence Livermore's National Ignition Facility (NIF), rely on finely calibrated optics for accuracy. The lenses, mirrors, and crystals that make up a laser's optical system serve various functions, from guiding a beam toward a reflective surface to correcting distortions. NIF's 192-beam system includes tens of thousands of optics that amplify and focus energy for hundreds of shots every year. In the high-energy-density regimes of these experiments, optical integrity is paramount.

Compromised optics are an expensive liability for laser performance. Debris and other damage initiators, also called precursors, can affect optical surfaces through laser-material interactions and subsequent material response, including etching, pitting, cracking, and melting. Degradation can lead to delamination of protective coatings as well as distortion, diffraction, blocking, or scattering of the laser beam. The Laboratory's Optics and Materials Science and Technology (OMST) organization manages efforts to analyze damage

precursors, improve fabrication and processing, and repair flaws. (See *S&TR*, September 2011, pp. 17–19; January/February 2015, pp. 19–22; January/February 2016, pp. 21–23; and July/August 2016, pp. 12–15.)

Recently, a team of OMST scientists, with input from collaborators at Lawrence Berkeley National Laboratory and the University of Rochester's Laboratory for Laser Energetics, completed a project funded by the Laboratory Directed Research and Development (LDRD) Program to examine in detail coupling mechanisms between lasers and contaminants on optical surfaces. Livermore physicist Manyalibo (Ibo) Matthews led the project, which aimed to understand how contaminant particles interact with laser beams, how particle shape and particle-induced damage affect beam propagation, and how damage morphology evolves in the presence of high-energy lasers.

Wear and Tear

Like many sensitive instruments, optical components are susceptible to dirt, debris, and defects at all phases of their production and operation, including fabrication, processing, handling, and installation. In addition, airborne particles generated during laser operation or present in a laboratory environment can relocate to other areas, potentially contaminating optical surfaces.

Optics closer to the laser's target encounter additional threats. At NIF, a disposable debris shield positioned between the final optics and the target can begin to break down with use, potentially introducing glass shards and particulates into the optical field. In addition, during an ignition shot, the target (a gold hohlraum containing a deuterium–tritium fuel capsule) is compressed as its holder is blown apart, generating fragments that can threaten the nearest optics.

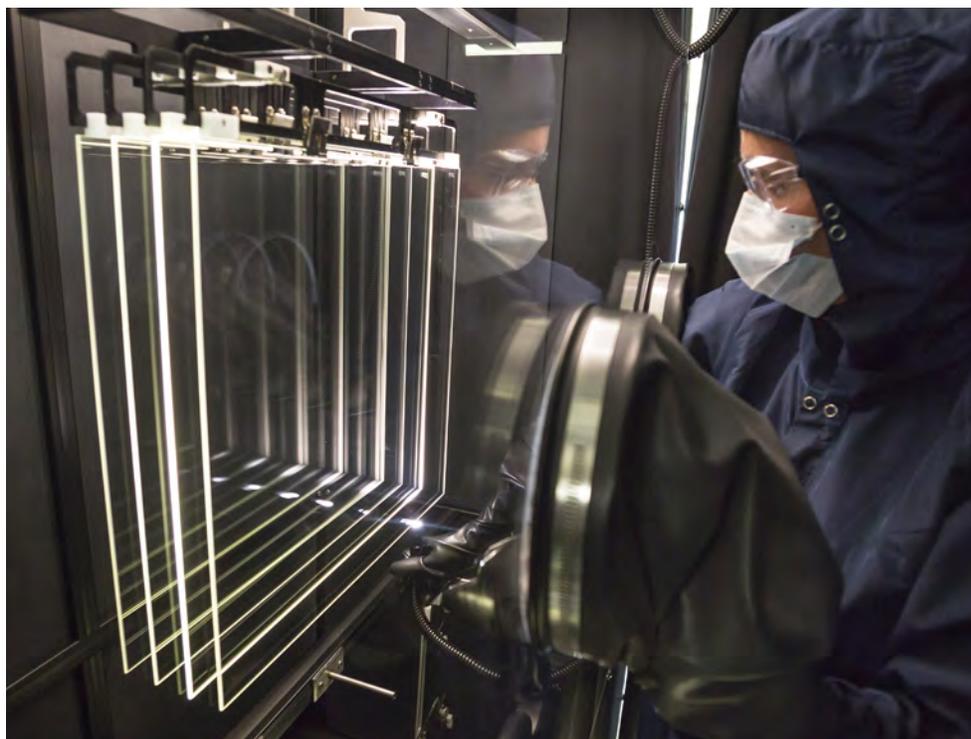
Besides sustaining damage from surrounding materials, optics are directly affected by the high-energy laser beams. Repeated exposure over time contributes

to accumulated defects. Furthermore, debris on the input side of an optical component can diffract incoming laser light, altering the beam path and promoting damage initiation on the exit side of the optic. Ironically, just as an attempt to clean eyeglasses might smear a substance across or grind particles into the lenses, dry laser cleaning—using a low-energy laser pulse to clear off debris—can also damage optics by creating shallow pits.

A Complex Approach

Matthews' LDRD team took a multifaceted approach to investigating the interaction of laser energy with micrometer-scale metallic and glass particles on optical surfaces. The researchers conducted experiments to measure particle velocity, plasma formation, and ejected material, and computer simulations were used to predict laser absorption and damage effects on beam propagation and performance. Livermore's robust diagnostic capabilities included a time-resolved imaging method that exposes nonuniformities in materials, and plasma emission spectroscopy, which measures spectral wavelengths of light generated during laser ablation of particles on optics.

Multilayer dielectric (MLD) coatings are an integral part of high-power laser systems for beam combination, beam steering, wavelength separation, and diffraction gratings. Team member Roger Qiu led tests to determine titanium particles' effects on the capping materials of MLD coatings. Titanium particles in general



At the National Ignition Facility, a low-cost disposable debris shield (several are shown here) protects the final optics from debris and contamination. However, the disposable shield is susceptible to damage, which, in turn, can cause glass shards and particulates to be introduced into the optical field.

can be generated in high-power pulsed-laser systems through laser ablation within beam dumps and the subsequent deposition of condensed metal vapor on nearby optics. By combining large-aperture laser damage testing, scanning electron microscopy, and numerical modeling, Qiu's team uncovered the responses of different capping materials on specific MLD mirror layers to laser-particle interactions. Qiu says, "The knowledge we gain from these experiments will guide new materials development to guard against laser-induced damage of MLD coatings."

Laser-induced pitting scatters the light from the laser and causes the optical surface to become hazy, but the team was not sure how problematic such effects were to overall laser performance. "We learned that metal contamination could cause shallow pits on the glass surface," explains physicist Eyal Feigenbaum, comparing the typical pit to the shape of a margarita glass. Feigenbaum created simulations of pit formation and morphology and developed models to characterize the resulting beam degradation. Further tests with large-aperture beams, in which large numbers of particles were evaluated simultaneously, enabled Feigenbaum to assess debris-caused damage characteristics.

A Range of Results

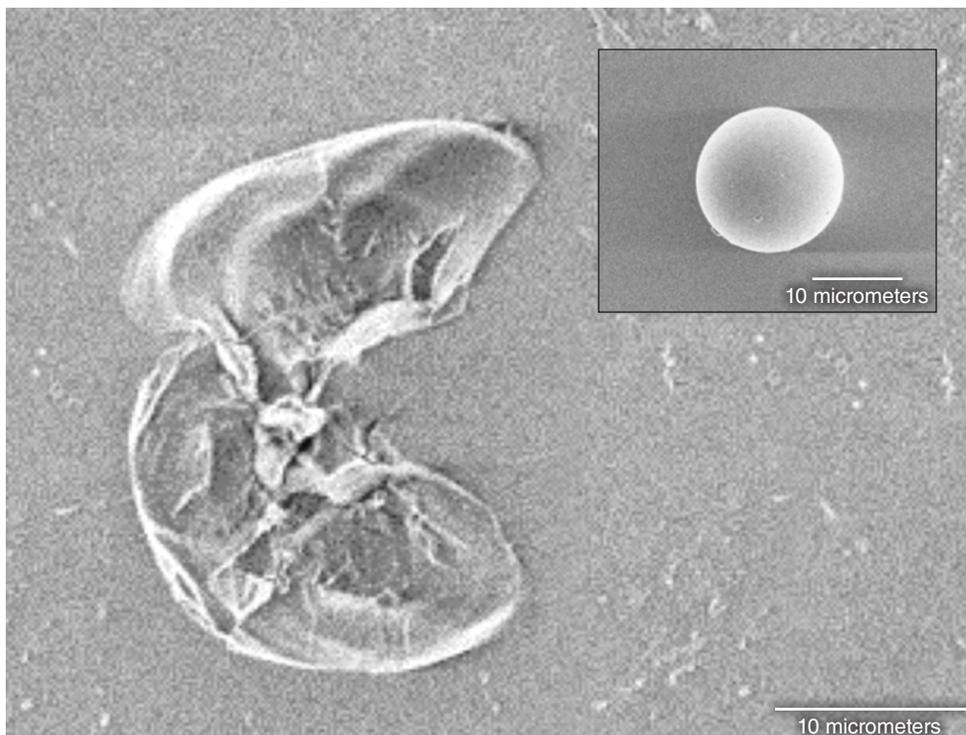
Matthews and colleagues found that the mechanisms governing laser-particle interactions depend on multiple factors. Regarding particle shape, the team saw a range of dispersal patterns following

a laser pulse. In some cases, the momentum of a beam hitting a spherical particle yielded a donut-shaped distribution of fragments. Irregularly shaped particles, such as those formed by mechanical abrasion, produced a shielding effect via dispersion fields that mimicked particle shape. In the MLD experiments, Qiu observed a relationship with the coatings' properties. He notes, "Contaminant-driven damage of MLD coatings is strongly dependent on the shape of particulates and the thermal expansion and mechanical strength of the coating materials."

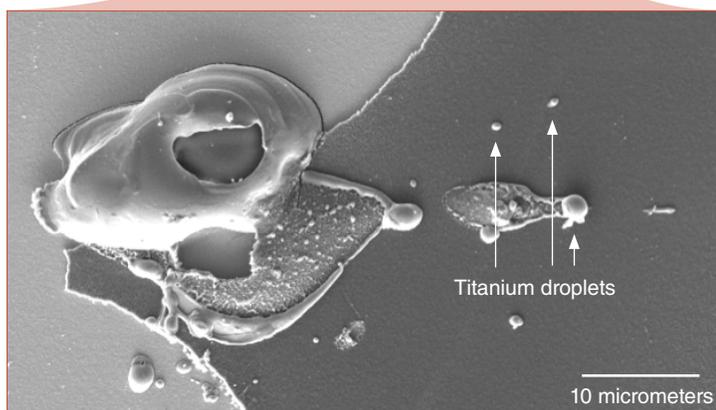
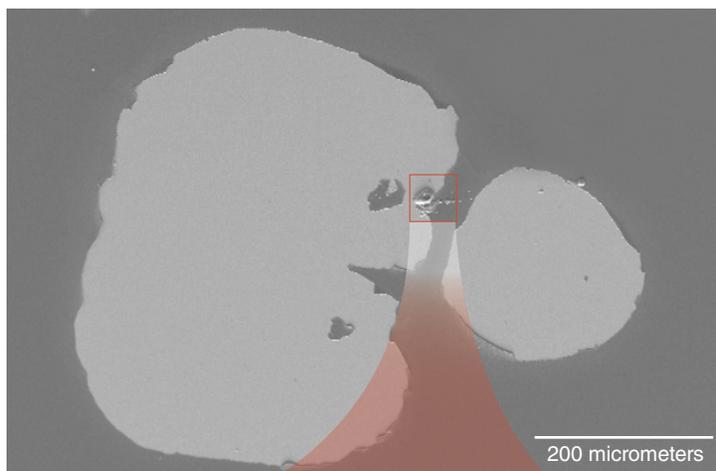
A particle's opacity also affects its behavior, as does the location of debris relative to the incoming beam. On an optical component's input surface, opaque particles tend to compress and disperse along the surface as the beam is obscured, whereas transparent particles tend to blow away from the substrate because more light energy is deposited into their interior. On the exit surface, the opposite occurs. Essentially, opaque particles are ejected while transparent particles break into shards and, under certain circumstances, fuse to the substrate, promoting damage initiation. Thus, opaque debris causes more damage on the input side, and transparent debris causes more damage on the exit side. These behaviors were key findings of the LDRD study.

The team's experiments and simulations also revealed interesting features of particle ejection and dispersion. Some particles move from one location on the optical surface to another without ejecting. Others disperse quickly or slowly depending on the intensity of beam fluence, and still other particles liquefy and spray out from the surface. Calculating particle velocity and trajectory helps estimate the strength of ejection mechanisms, including secondary effects such as shockwaves reverberating inside and breaking apart particles. "Ejected material has to go somewhere," observes Matthews. "These findings can inform upgrades to laser-ablation processes with a goal of removing ejecta from optical surfaces."

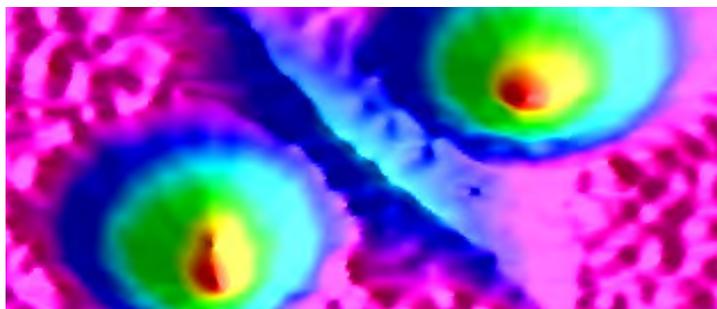
As energy transfers from the laser beam to the particle—a mechanism known as pulsed-laser momentum coupling—plasma forms between the surface and the



A scanning electron microscopy image shows damage on a fused-silica surface following laser irradiation of fragments left behind by an initial laser pulse irradiating a spherical borosilicate particle (inset). Glass fragments remaining on a pristine optic in high-power laser systems can lead to catastrophic damage if left untreated.



Scanning electron microscopy images show damage to a multilayer dielectric surface contaminated with titanium particles. (inset) A close-up view reveals the surface's complex morphology and indicates the formation of molten titanium droplets.



A false color, three-dimensional rendering shows two laser-induced shallow pits (LSPs) on a silicon-dioxide optical surface. A cluster of LSPs also creates the linear-like groove in the center. Typical dimensions for LSPs are up to a few tens of micrometers in width and hundreds of nanometers in depth.

particle. Matthews' team studied the shockwave generated by the laser and the resulting plasma plume. They found that different types of particles vary in their reaction to the shockwave, and plasma flow changes as the particle moves. By measuring the speed and temperature of plume formation, the team showed that plasma is sensitive to laser fluence, wavelength variations, and beam angle.

As for pits carved by metallic particles, Feigenbaum observed surprising behavior. "These shallow pits do not tend to grow with subsequent laser shots, so their effect is limited." But when the laser fires at higher energies, he warns, "Another mechanism kicks in, and deeper surface fractures are created. These fractures do grow with subsequent laser shots and limit an optic's lifetime." This relationship between beam intensity and pit and fracture formation allows scientists to evaluate beam-scattering effects on the system's performance. "The scattering model for the hazed-glass surface has been instrumental to operations and usability of NIF laser optics," says Feigenbaum.

Damage Control

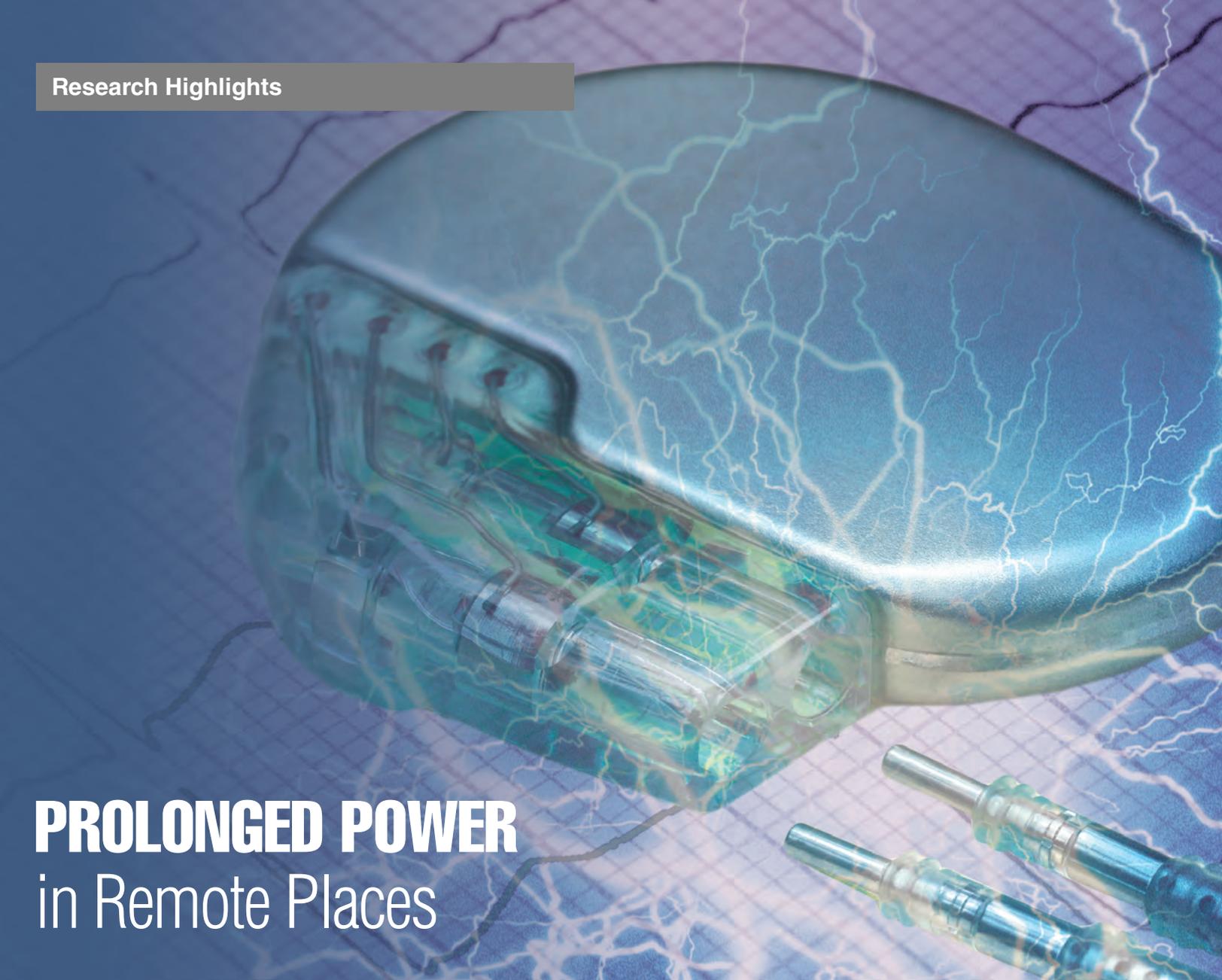
In keeping with the spirit of the LDRD Program, the team's experiments serve a larger purpose of innovation in optical design and laser performance. Understanding laser-matter interactions can inspire design improvements, such as vapor chemistry treatments, to make optics and coatings more impervious to damage or repellant to debris. Scientists can use these data to develop debris-removal techniques without compromising optical integrity and to enhance the Laboratory's computational capabilities to better predict contamination scenarios and prevent overuse. Cost savings naturally follow life-extension efforts.

Livermore's Directed Energy Program is poised to reap the benefits of this LDRD project in developing new types of laser technology, such as continuous wave and diode-pumped alkali lasers. Matthews also cites industrial settings in which optical surfaces play an important role, such as in lasers used to generate patterns or for machining materials with holes. He also recognizes the value of his team's findings for the next-generation of durable optical elements. He states, "Continuing our efforts to understand and control laser damage in high-power laser systems is crucial to maintaining NIF and supporting our missions for the National Nuclear Security Administration."

—Holly Auten

Key Words: debris, high-power laser, Laboratory Directed Research and Development (LDRD) Program, National Ignition Facility (NIF), optic, optical damage, optical system, Optics and Materials Science and Technology (OMST) organization, particle, plasma formation, surface contamination.

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PROLONGED POWER in Remote Places

A compact battery that provides long-lasting, reliable power without a tether to an electrical outlet could change the way people use electronics, from personal mobile phones to pacemakers. Three-dimensional (3D) radioisotope batteries—high-density power sources that convert a radioisotope’s radioactive decay directly into electricity—hold promise in devices suited for remote applications, such as unattended sensors, and for biomedical purposes. The development of 3D radioisotope batteries relies on the skill of experts at Lawrence Livermore, whose knowledge of advanced microfabrication, materials science, and nuclear chemistry are propelling the technology forward.

Although radioisotope batteries have existed for decades, they tend to be expensive to produce and have relatively low power levels, which limits their output. To create long-lasting battery options suitable for a broader range of power and lifetime requirements, a Livermore team led by electrical engineer

Rebecca Nikolic has demonstrated a two-dimensional (2D) radioisotope battery with properties intended for 3D construction. As part of the research, the team is testing semiconductor materials for radiation hardness—how resistant they are to damage from ionizing radiation. They are also developing radioisotope coatings that emit beta or alpha particles. These particles then deposit energy into the semiconductor material to generate electricity.

The team’s work builds on a previous project, initially funded by Livermore’s Laboratory Directed Research and Development Program, to develop a silicon pillar-based radiation detection device, which contains millions of etched pillars 50 micrometers high and spaced approximately 2 micrometers apart. (See *S&TR*, March 2014, pp. 12–15.) “Our team has taken this platform, which took a decade to develop, and is now exploring new applications,” says Nikolic. “We are excited about the possibilities.” The pillar platform is a starting point

for developing the 3D radioisotope battery, a device that would have a greater power density than a flat, 2D material because it can house a larger volume of the radioisotope.

Architectural Considerations

Radioisotopes can vary in level and type of energy they produce, which correlates with the amount of radiation they emit. They also have different half-lives, a characteristic that dictates how long the radioisotope will generate energy, and thus ultimately determines how long a radioisotope battery will last. Tritium is a low-energy, beta-emitting hydrogen radioisotope that produces less than 10 kiloelectronvolts (keV) of energy per decay. Tritium-based beta-emitting (or beta-voltaic) batteries are the most commonly made radioisotope batteries because they are relatively low power yet long lasting.

Livermore found success developing a higher energy prototype battery using promethium-147, a beta-emitting radioisotope that produces a mean energy of 62 keV. “Leveraging promethium-147 in our batteries has furthered the ability to have a higher power density compared to many other beta-voltaics,” explains Nikolic.

Alpha-emitting (alpha-voltaic) radioisotopes can generate up to approximately 5 megaelectronvolts (MeV) and typically give off about 1,000 times higher power than most beta-emitting ones. However, energy at such levels can damage a crystalline semiconductor and its surrounding electronics. Therefore, alpha-voltaic batteries are sought after for high-power applications, but are difficult to make because the battery materials must withstand large radiation doses.

A second consideration is the semiconductor itself, which captures the radiation, creates the electrical charge, and then transports the charge to an electrode. The Livermore team designed a beta-voltaic battery prototype in which 3D silicon carbide pillars were surrounded with promethium-147. With this design, the researchers showed that silicon carbide is a viable semiconductor material for the 3D pillar structure of



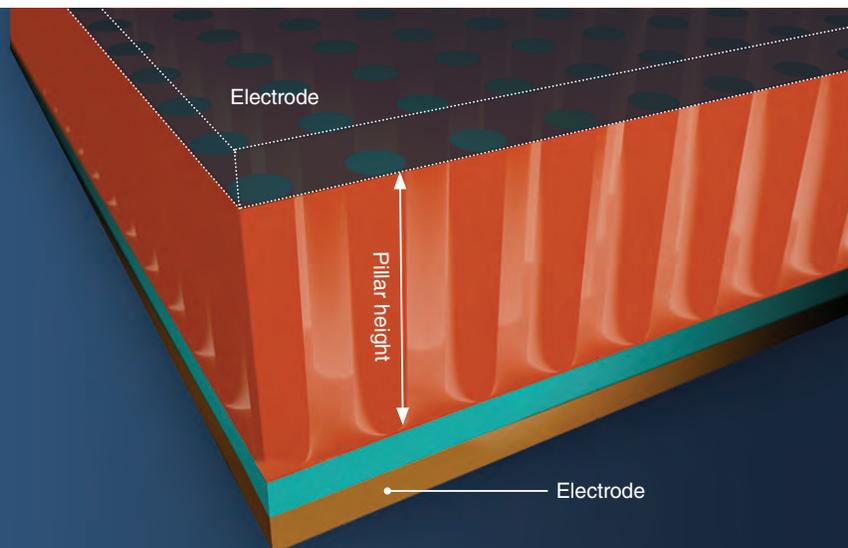
Livermore materials scientist Lars Voss holds a vial containing selenium-iodine. This semiconducting material may be useful for developing long-lasting, reliable radioisotope batteries. (Photo by Randy Wong.)

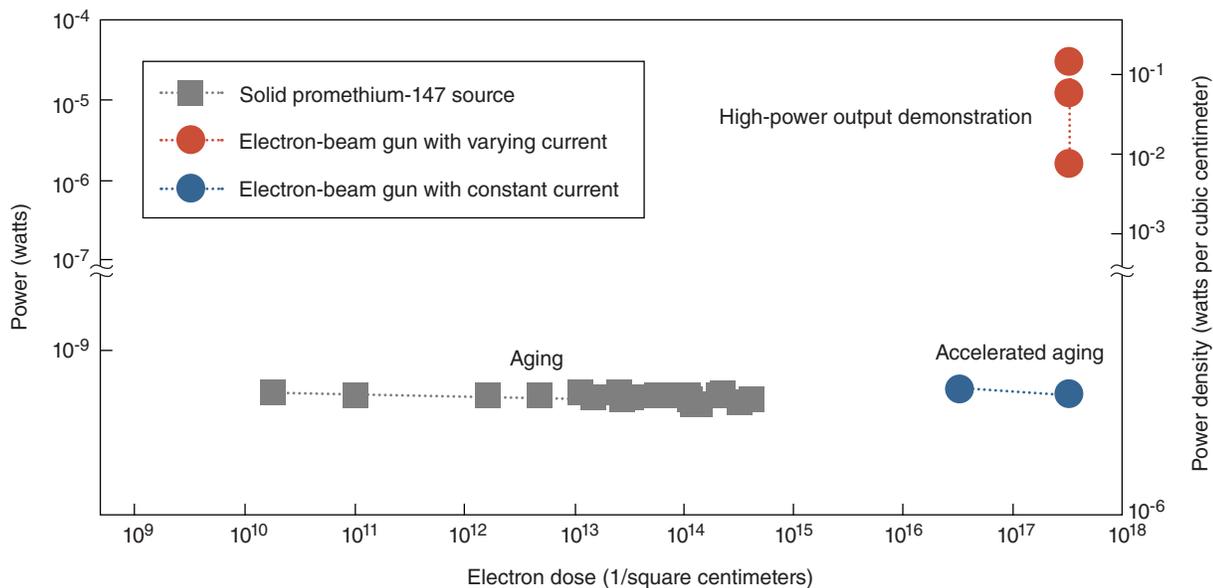
beta-voltaic batteries up to at least 62 keV. However, beta- and alpha-emitting radioisotopes above 1 MeV would destroy the crystal lattice of silicon carbide and other hard materials, presenting a clear need for a radiation-resistant semiconductor.

A Game Changer

In its liquid form, the semiconducting material selenium is reported to be resistant to radiation damage because liquids have a noncrystalline structure. However, selenium only remains in its liquid form at temperatures above 220 degrees Celsius, high enough to damage the surrounding materials within the battery and the local area. The team found that adding iodine to selenium significantly lowers its melting temperature without inhibiting the semiconductor’s performance—that is, no change in its performance was

The Livermore-developed three-dimensional radioisotope battery design features pillars made from silicon carbide surrounded by a radioisotope, such as promethium-147.





observed when transitioning from solid to liquid selenium. For instance, a mixture of equal parts selenium and iodine has a melting point of just 57 degrees Celsius, a more practical temperature for a battery.

The selenium–iodine semiconductor mixture may be radiation hard, making the mixture potentially useful for both low- and high-energy beta- and alpha-voltaic batteries. In a selenium-based battery, the radioisotope could be part of the liquid mixture as opposed to a coating. “Liquid-selenium-based batteries may be impervious to damage,” says Lars Voss, a Laboratory materials scientist. “This finding could be a game changer for radioisotope power sources and enable far higher power densities with far lower radioactivity.”

Test of Time

A reliable radioisotope battery must be durable. Toward this end, the Livermore team has studied how radiation exposure affects the semiconductor material over time. The most efficient way to perform this task is through accelerated aging techniques—a core competency developed at the Laboratory for stockpile stewardship.

Experiments were conducted using a new electron-beam gun, tunable to the required energy levels of 0 to 100 keV. The source generates a beam of electrons, which act as surrogate beta particles, tunable to the energy level of the radioisotope. As the semiconductor material is irradiated by the beam, the team monitors the material over time to determine its electron dose. These data indicate how long the material can withstand radiation exposure, which correlates with the lifespan of a battery. Using the electron-beam gun, the team can subject the

The team studied how radiation exposure affects the behavior of a radioisotope battery's semiconductor material, both with a solid promethium-147 source up to an electron dose of 10^{15} and with an electron-beam gun tuned to 62 kiloelectronvolts to simulate higher doses.

target material to many years' worth of radiation exposure in just one hour, reducing experiment time and cost. Data from these studies are being used to refine the battery design.

Pumping Up to 3D

The Livermore team has produced promising results for both beta- and alpha-voltaic battery designs. The researchers' next steps will involve further refining battery properties and applying their findings to the silicon-carbide 3D structure. Additional research efforts will help the team improve its fundamental understanding of liquid semiconductors.

The advent of this radioisotope battery has the potential to benefit other work at Lawrence Livermore, much like its 3D radiation-detection predecessor did. Nikolic says, “When we complete the 3D radioisotope battery, it's going to find a home in many applications.”

—Lanie L. Helms

Key Words: accelerated aging, alpha-voltaic battery, beta-voltaic battery, pillar, power, promethium-147, radiation, radioisotope battery, silicon carbide, selenium, semiconductor.

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In this section, we list recent patents issued to and awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory. For the full text of a patent, enter the seven-digit number in the search box at the U.S. Patent and Trademark Office's website (<http://www.uspto.gov>).

Patents

Adaptive CT Scanning System

Stephen E. Sampayan
U.S. Patent 9,500,601 B2
November 22, 2016

Nuclear Radiation Cleanup and Uranium Prospecting

Raymond P. Mariella, Jr., Yves M. Dardenne
U.S. Patent 9,533,334 B2
January 3, 2017

Nanodevices for Generating Power from Molecules and Batteryless Sensing

Yinmin Wang, Xianying Wang, Alex V. Hamza
U.S. Patent 9,537,157 B2
January 3, 2017

Post Polymerization Cure Shape Memory Polymers

Thomas S. Wilson, Michael Keith Hearon, II, Jane P. Bearinger
U.S. Patent 9,540,481 B2
January 10, 2017

Awards

Lawrence Livermore physicist **Manyalibo (Ibo) Matthews** has been elected a fellow of the **Optical Society (OSA)**. He was recognized for his “outstanding contributions and sustained leadership in the field of high-power laser-induced damage science, laser–material interactions, and processing and vibrational spectroscopy–based materials characterization.” Matthews joined the Laboratory in 2006 and serves as the deputy group leader for Optical Materials and Target Science in the Materials Science Division of the Physical and Life Sciences Directorate.

OSA fellows are selected on various criteria, such as a record of significant publications or patents related to optics, achievements in optics, management ability, and service to OSA or the global optics community. The number of OSA fellows is limited to less than 10 percent of the total OSA membership, and the number elected each year is less than 0.5 percent of the current membership total.

John Taylor, former Livermore group leader for Precision Engineering, was presented with the **American Society for Precision Engineering's (ASPE's) Distinguished Service Award** for his continued dedication to supporting fellow engineers. He was honored for his efforts in shepherding technologies that he believed were essential for the country and in maintaining the vitality of the organization. Taylor has served as the director-at-large, secretary, vice president, and president of ASPE during his 31-year membership with the society.

A Lawrence Livermore team's dramatically improved first-principles molecular dynamics code that promises to enable new computer simulation applications was one of the finalists for the **2016 Gordon Bell Prize**. The team, which included lead **Jean-Luc Fattebert** and members **Daniel Osei-Kuffuor, Erik Draeger, Tadashi Ogitsu, and William Krauss**, presented its groundbreaking project at the 2016 Supercomputing Conference (SC16).

Molecular dynamics has become one of the principal methods for studying the movement of atoms and molecules in complex systems

and has broad application in chemistry, physics, materials science, biology, and medicine. The team's project was initially funded by Livermore's Laboratory Directed Research and Development Program and continues to be supported through the Department of Energy and the National Nuclear Security Administration.

The **Greenhouse Gas Control Technologies** conference series has awarded Lawrence Livermore's **Samuel (Julio) Friedmann** with a **Greenman Award**. Friedmann was recognized for his tireless efforts to promote carbon capture and storage, particularly at large scale. This award is given to those who have made career-scale impact on the management of carbon dioxide removal, storage, and utilization.

Friedmann serves as the senior advisor for Energy Innovation at the Laboratory and is working with high-level managers on Mission Innovation—a flagship initiative to dramatically accelerate the development and deployment of clean energy innovations.

Lawrence Livermore National Laboratory has been honored with a **Gold 2016 Optimas Award** for Recruiting from **Workforce Magazine**. The award recognized the Laboratory for excellence in its military internship programs, specifically, the Military Academic Research Associates program, the ROTC (Reserve Officers' Training Corps) Internship program, and the Newly Commissioned Officer program.

Workforce Magazine bestows the Optimas awards each year for human resources and workforce management initiatives that achieve business results. Management professionals nominate their own initiatives, which are then chosen by the magazine's editors. Optimas awards are given out in multiple categories. The recruiting award honors organizations that have developed and implemented an innovative and effective recruitment initiative that helped the organization source, attract, and recruit job candidates.

Investing in the Nation's Future

For more than a quarter century, the Department of Energy's Laboratory Directed Research and Development (LDRD) Program has made possible transformative scientific and technological solutions to ever-changing national security challenges. Under LDRD, the Laboratory invests 6 percent of its operating budget (about \$87 million in fiscal year 2017) in areas beyond the scope of programmatic research and where high-risk research could lead to big payoffs. As the primary source of discretionary research and development funding at the Laboratory, the program helps to maintain the vitality of Livermore science and technology relevant to national security. The most innovative science and engineering programs at Livermore often have roots in LDRD. Projects sponsored by the program contribute significantly to intellectual property, publications, and collaborations. The technical output of LDRD researchers—patent disclosures, peer-reviewed publications, and publications cited by other authors—typically accounts for one-quarter of the Laboratory's total. In the last 10 years, some 60 percent of Livermore's R&D 100 awards have been attributed to LDRD. In addition, many technologies that come out of the LDRD Program are licensed to the private sector to strengthen U.S. industry. Among the most valuable aspects of the program is its role as an outstanding tool for professional growth and recruitment.

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Ready, Set, Innovate!



Guiding entrepreneurs through successful technology transfer is a key objective for Livermore's Industrial Partnerships Office.

Also in June

- *A new Department of Energy program educates budding scientist-entrepreneurs about business practices to foster technology transfer.*
- *Livermore simulation experts have constructed a version of a powerful engineering and physics computer code for U.S. industry and universities.*
- *Laboratory researchers use chemistry, engineering, and computational expertise to develop a new manufacturing technique for high-performance composites.*

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